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Production of Sustainable Aviation Fuels from Lignocellulosic Residues in Brazil through Hydrothermal Liquefaction: Techno-Economic and Environmental Assessments

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Abstract: Decarbonization of the aviation sector relies on deployment of sustainable aviation fuels (SAF) at commercial scale. Hydrothermal liquefaction (HTL) has been recognized as a promising technology to help supply the increasing projected SAF demand. High availability of agro-industrial residues, combined with a well-established biorefinery system, makes the sugarcane industry in Brazil a good option for HTL technology deployment. Moreover, challenges regarding the economic feasibility of SAF from HTL could be partially addressed by the RenovaBio policy, a market-driven incentive mechanism of carbon credits implemented in Brazil. This study investigated both the techno-economic and life cycle assessment of SAF production from sugarcane lignocellulosic residues, considering HTL integrated to a first-generation ethanol distillery and a HTL stand-alone facility. The evaluated scenarios showed great climate mitigation potential, reaching a reduction of up to 73–82% when compared to fossil jet fuel. The minimum fuel selling price of SAF at 15.4 USD/GJ indicated potential of economic competitiveness with fossil jet fuel in the best integrated scenario. The economic benefits obtained from carbon credits are not enough to enable feasibility of HTL in the stand-alone scenarios, even with carbon prices projected at 125 USD/tonne CO_2-eq avoided.

Keywords: biorefinery; climate change mitigation; life-cycle assessment; advanced biofuels; bagasse; sugarcane residues; biokerosene; RenovaBio; Cbios

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1. Introduction

The global climate emergency has prompted worldwide efforts to accomplish net-zero emissions in order to limit the long-term rise in average global temperatures to 1.5 °C [1]. A recent study by International Energy Agency (IEA) [2] showed that electricity is to become dominant in the transport sector by 2050 to achieve a net-zero emission scenario. However, the electrification of the aviation sector presents some challenges, mainly associated with aircraft fleet replacement, in addition to limitations regarding battery energy density. This report issued by IEA highlighted the pivotal importance of synthetic liquid fuels and advanced biofuels for the decarbonization of the aviation sector worldwide. Moreover, SAF demand is projected to have a share of 45% of the total aircraft fuel consumption by 2050. This projection is in line with the prospects of the European Parliamentary Research Service, which recognized sustainable aviation fuels as having the most significant potential for emission mitigation of the aviation sector in the short term. In fact, there is an undergoing aviation initiative in Europe, ReFuelEU [3], which proposes mandatory blending of sustainable aviation fuel (SAF) into fossil jet fuel to be provided at major airports in the EU, with an increasing SAF share of 2% by 2025, until it reaches 63% by 2050. In the same sense, the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) set a goal of carbon neutral growth from 2020 onwards for international civil aviation. This demand requires an offset of about 2.5 billion tonnes of CO_2 between 2021 and 2035 worldwide [4]. Moreover, their offsetting requirements will be mandatory from 2027 onwards for all international flights (with a few exceptions). Of the seven pathways to produce SAF that have already been certified by ASTM D7566, hydroprocessed esters and fatty acid synthetic paraffinic kerosene (HEFA-SPK) is the one with the most advanced technology readiness level and is in commercial use [5,6]. The blending ratio of SAF with fossil jet fuel depends on the feedstock and production pathway. Although the maximum certified blend ratio is 50%, the current blends for commercial flights are still at a low baseline of 1%. For instance, the airline company KLM is currently adding 1% of SAF blend in all their commercial flights departing from Amsterdam Airport Schiphol, and intends to reach a 10% blend ratio by 2030 [7]. The same goal of a 10% SAF blend with fossil jet fuel in commercial flights by 2030 was reported by Delta Airlines [8]. Despite increasing commitment of the aviation sector towards decarbonization, the current SAF production corresponds to less than one percent of jet fuel demand [5]. This only highlights the importance of the deployment of technologies such as HTL at large scale, to help supply the growing demand for SAF expected in the next years.

Brazil is also making efforts towards an effective decarbonization in the transport sector. The Brazilian National Biofuel Policy, known as RenovaBio, is a market-driven incentive mechanism of decarbonization credits, called Cbios. This program was launched in 2017, aiming to reduce the carbon intensity of the Brazilian fuel matrix. It is expected that the implementation of the RenovaBio policy will generate investments in the Brazilian biofuels sector in the order of USD 2.4 billion [9]. These investments and carbon reduction incentives may be critical for the establishment of biofuel technologies which are not available on the market, given that a very significant share of reductions in the GHG emissions are expected to rely on technologies that are still in the demonstration phase [2]. Within the technologies that are able to convert residues with a low carbon footprint into sustainable aviation fuels, hydrothermal liquefaction (HTL) stands out as having very appealing potential [10–12]. HTL demonstration plants are already in operation and some of them have started licensing their technologies envisioning commercial exploitation [13,14]. Furthermore, HTL has been widely recognized as a high feedstock-flexibility process with the ability to deliver relatively high conversion yields [10,15–20]. Studies have pointed out that SAF produced via HTL can reduce lifecycle GHG emissions by up to 85% compared to fossil jet fuel [11,21,22]. Despite this promising potential, there is a lack of studies that jointly evaluate the economic and environmental performances of SAF from HTL, particularly in the Brazilian context.

Feedstocks with low carbon footprint are vital to the production of sustainable aviation fuels. The Brazilian sugarcane industry possesses high availability of agro-industrial residues, along with a very well established biorefinery system. The implementation of HTL technology within a first-generation ethanol plant could benefit from energy integration (shared utilities) and from the additional revenues from ethanol commercialization [23,24]. Nevertheless, the potential for carbon mitigation of HTL technology integrated into the sugarcane industry to produce SAF has not yet been investigated. The trade of Cbios within the scope of RenovaBio could help strengthen SAF production to supply the increasing demand for the next decades. Regarding technical aspects of HTL, a substantial number of articles have investigated the advantages of using organic solvents such as ethanol to improve HTL bio-crude yield and quality. They claimed that this utilization would not cause environmental issues when derived from renewable sources [25–28]. No study in the literature has investigated the environmental impacts of deploying ethanol, instead of water, as a liquefaction solvent at industrial scale. Another aspect that deserves attention when it comes to the production of SAF is the need for hydrogen in the upgrading of bio-crude oil. Hydrogen can be purchased or produced in situ through steam-methane reform (SMR) or through cleaner alternatives, in which the production pathway will have a direct impact on GHG emissions of SAF [21,22,29]. Most assessments concerning HTL have proposed in situ production of hydrogen to supply the hydrotreatment unit, where the description of hydrogen production is detailed in [30–36]. The ethanol distillery produces a considerable amount of vinasse, which is usually utilized for fertirrigation purposes. This vinasse could be subjected to biodigestion, and the obtained biomethane converted into hydrogen through SMR, avoiding the use of natural gas feedstock.

The present study aimed to evaluate the techno-economic and environmental performance of SAF production through a HTL facility integrated into the Brazilian sugarcane industry. The production of anhydrous ethanol considering the state-of-the-art technology in Brazilian biorefineries is described in detail in previous works [23,37–47]. The sugarcane sector produces an abundant amount of residues and their conversion into SAF could help meet the mitigation targets established by national and international instruments such as RenovaBio and CORSIA. HTL as a stand-alone facility is also covered in this study to better understand the trade-offs between these two different industrial configurations, as well to simplify the comparison between the obtained results and the literature results. This research provides a unique contribution, since there is no study in the literature, either examining a stand-alone or an integrated configuration, that concomitantly undertakes a thorough analysis of the economic and environmental aspects of SAF production from sugarcane bagasse and straw via HTL with different liquefaction solvents. Another novelty of the present study is the evaluation of the biodigestion of vinasse to provide a clean and renewable source of biomethane for in situ hydrogen production for the upgrading of HTL bio-crude oil. Moreover, a risk analysis is undertaken to understand the uncertainties associated with the key variables of the process, and their influence on the results. This study is structured as follows. The methodology is delineated in Section 2, where the evaluated scenarios are described along with the adopted premises and data source for the techno-economic analysis, the life cycle assessment, and the risk analysis. In Section 3, the main economic and environmental metrics obtained in this study, such as the minimum selling price and the GHG emissions of SAF, are presented and discussed, taking into consideration the results of the uncertainty analysis. A comparison of the obtained results with the literature is proposed, and the implications of carbon price projections for the viability of the investigated scenarios are presented. Finally, Section 4 discusses the main findings of the study and concludes with a few recommendations.

2. Materials and Methods

2.1. Scenarios Description

To understand the environmental impacts related to the production of SAF through HTL in Brazil, five biorefinery scenarios were evaluated, within two technological configurations: stand-alone (SA) and integrated (INT). In the assessed scenarios, different biomasses and liquefaction solvents were considered. Within the SA configuration, the conversion of sugarcane bagasse (SCB) with water (SA-H_2O_SCB) and ethanol (SA-EtOH_SCB) was evaluated, as well as the conversion of straw (STW) with water (SA-H_2O_STW). Within the integrated configuration (HTL plant integrated into an ethanol distillery), the scenarios assessed the conversion of bagasse and straw with water (INT-H_2O_SCB&STW) and bagasse and straw with ethanol (SA-EtOH_SCB&STW). The utilization of ethanol as solvent for liquefaction reactions was evaluated in only one case for each of the industrial configurations. This is due to the fact that in a previous study [48] the use of ethanol as solvent showed no evidence of economic viability, but the environmental performance of this input at an industrial scale has not yet been investigated in the literature. In the integrated scenario (INT-EtOH_SCB&STW) ethanol is diverted from the ethanol distillery to the HTL plant to be used as solvent medium in the liquefaction process. The description of the evaluated scenarios is shown in Figure 1.

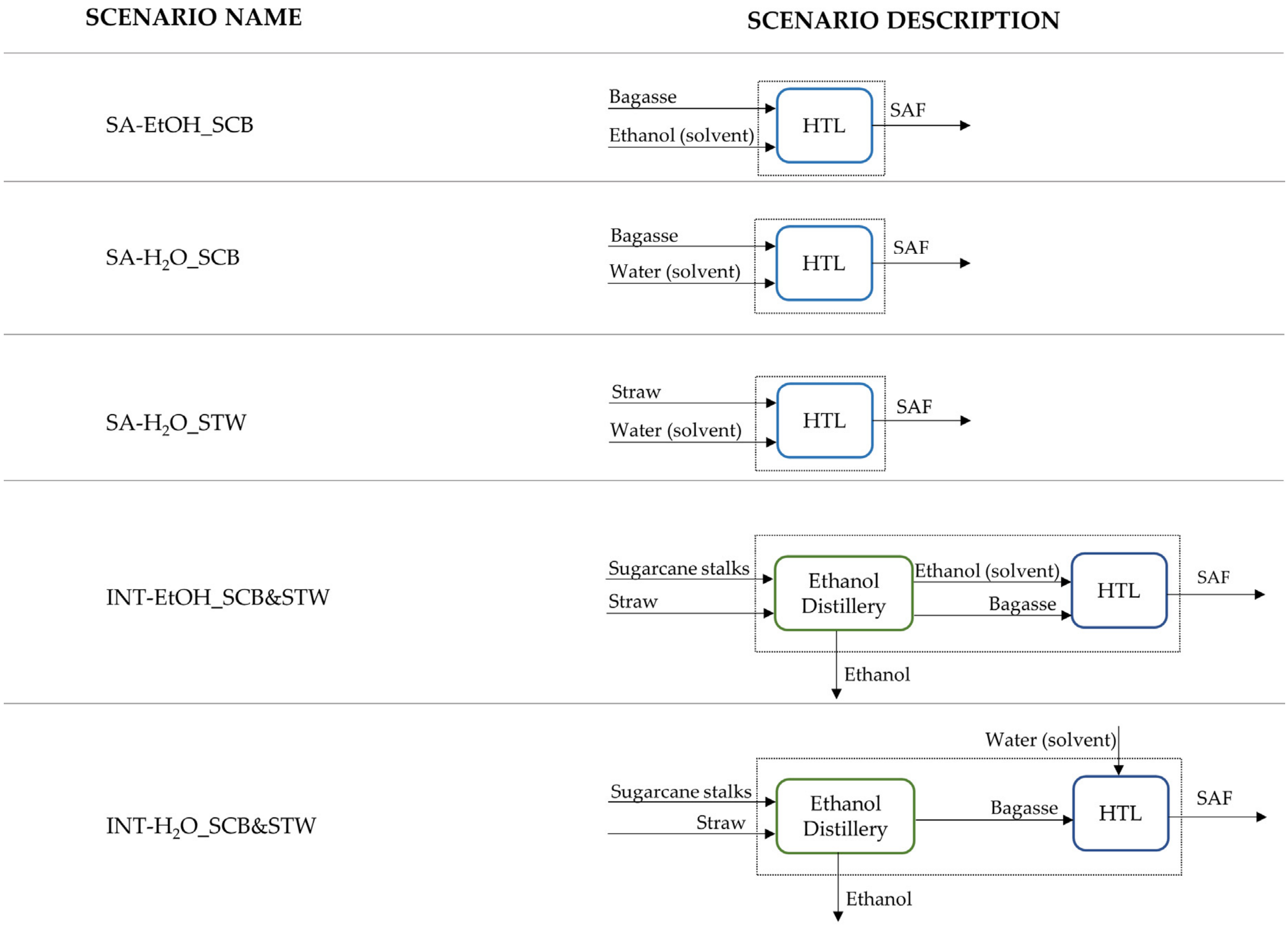


Figure 1. Simplified fluxograms of the proposed scenarios. Solvent varies according to each scenario: for SA-EtOH_SCB, the solvent is anhydrous ethanol (purchased from surrounding mills) and for the INT-EtOH_SCB&STW scenario, ethanol is diverted from the distillery that is integrated into HTL plant. For the SA-H_2O_SCB, SA-H_2O_STW, and INT- H_2O_SCB&STW scenarios, the solvent is water.

2.2. Process Description

2.2.1. Biomass Production Systems

The production costs of the sugarcane stalks and straw were calculated with the aid of an existing assessment tool, called CanaSoft, developed within the Virtual Biorefinery (VB) framework [49]. CanaSoft consists of a spreadsheet model that calculates the technical, economic, and environmental impacts of the whole agricultural production system. It includes the pre-planting, planting, cultivation, and harvesting operations. The agricultural stage was modeled following the same premises of a previous work [48]. The main parameters adopted for the biomass production system, as well as the outputs calculated by CanaSoft, are shown in Table 1. As the sugarcane bagasse, an industrial residue that remains after juice extraction in sugarcane mills is usually burned in boilers to produce electricity, the bagasse opportunity costs were retrieved from the Sugarcane Renewable Electricity Project developed in Brazil [50].

Table 1. Main parameters adopted for the biomass production system.

Parameter	Value	Unit	Reference
Mill crushing capacity	4	Million t	[49]
Sugarcane productivity yield	80	t/ha/year	[49]
Number of cuts per cycle	5	-	[42]
Straw recovery fraction [a]	50	%	[50]
Straw recovery method	Bales	-	Assumed
Mean transportation distance [b]	36.1	km	Calculated
Sugarcane stalks production cost	22.0	USD/t	Calculated
Sugarcane straw production costs	27.2	USD/t	Calculated

[a] Straw recovery adopted considering previous recommendation to maintain soil quality [50]. [b] Calculated with CanaSoft model.

2.2.2. Stand-Alone Configuration: Hydrothermal Liquefaction Plant

The hydrothermal liquefaction plant processes either sugarcane bagasse or sugarcane straw. The plant processes 1124 dry metric tons of lignocellulosic material per day in 330 days of operation per year. The biomass is processed as received, without drying. The mass and energy balances for the HTL stage were calculated based on the data of heat, electricity, and material inputs and outputs of previous studies [12,51–53] with reliable data on the HTL technology. More details on the HTL industrial stage can be found in a previous study [48] and in the Supplementary Material (Table S2). The main technical parameters are listed in Table 2.

Table 2. Main parameters adopted for the HTL plant.

Parameter	Unit	Ethanol	Water	Reference
Scenario description				
Bagasse feed rate	dry t/day	1124	1124	Calculated
Straw feed rate	dry t/day	1124	1124	Calculated
Biomass moisture	%	50	50	[49]
Straw moisture	%	15	15	[49]
Operational days	day/year	330	330	[49]
Liquefaction				
Biomass-to solvent ratio	wt.%	20/80	20/80	Assumed
Reaction temperature	°C	300 °C	300 °C	[25]
Bio-crude yield, of dry feed [a]	wt.%	48.3	40.9	[25]
Heat exchange efficiency	%	80	80	Assumed
Upgrading				
Conversion temperature	°C	400	400	[12]
H_2/bio-crude ratio	kg H_2/kg BCO [b]	0.035	0.035	[12]
LHSV 1st stage FBR [c]	$v/v/h$	0.54	0.54	[12]
LHSV 2nd stage FBR	$v/v/h$	0.18	0.18	[12]
Products distribution				
Deoxygenated oil	wt.%	75	66	[12]
Water	wt.%	18	27	[12]
Off-gas	wt.%	7	7	[12]
Distillation output streams				
Gasoline	wt.%	30	30	[54]
Diesel	wt.%	15	15	[54]
Jet fuel	wt.%	50	50	[54]
Marine fuel	wt.%	5	5	[54]

[a]: Bagasse and straw are regarded to produce the same yield of bio-crude oil; [b]: Bio-crude oil; [c]: Fixed bed reactor.

2.2.3. Integrated Configuration: Ethanol Distillery with Hydrothermal Liquefaction Plant

The conversion of sugarcane into ethanol was modeled according to a previous study [48]. The distillery produces anhydrous ethanol (99.6 wt.%) and the surplus electricity is sold to the grid. The ethanol distillery operates during the sugarcane season

(200 days/year). The combined heat and power (CHP) unit provides steam and electricity for the ethanol distillery and for the HTL plant. The CHP is fueled with sugarcane bagasse and straw. The surplus of bagasse (not used to supply the demand for utilities) is sent to HTL conversion. The simulations related to the industrial stage of ethanol production were obtained with the aid of VB platform. More detailed information is available in previous publications based on this framework [49]. Additionally, the present study considered biodigestion of vinasse to supply the methane used for hydrogen production. The parameters for the vinasse biodigestion process are described in previous studies [55,56].

2.3. Techno-Economic Analysis

The economic assessment was performed by means of the discounted cash flow analysis. The economic viability of the evaluated scenarios was assessed using representative metrics such as net present value (NPV) and internal rate of return (IRR). The minimum attractive rate of return (MAAR) adopted for this study was 12% per year, based on the average interest rate used for projects related to the sugarcane industry in Brazil. [40].

The capital costs of the ethanol distillery were calculated based on the database available in VB platform. The CAPEX of HTL plant was calculated based on literature data [12], which were adjusted according to location factor, inflation rates in Brazil, and the reference date. Capital costs scaling parameters were the same as those used by Deuber et al. [48] and are detailed in the Supplementary Material.

Biomass costs were calculated using the CanaSoft model, as explained in Section 2.2.1. Other operational costs, including equipment maintenance, chemicals, and wages were calculated following the same premises as those described in Deuber et al. [48]. The selling prices of the fuels were obtained from the National Agency of Petroleum, Natural Gas and Biofuels [57], and estimated based on the last ten-year-average of historic data. Inflation effects were accounted for using Brazil's General Price Index-Market (IGP-M) and converted to USD based on the exchange rate in December 2019. Table 3 shows the main parameters adopted in the techno-economic analysis.

Table 3. Main parameters used in the techno-economic analysis of integrated and stand-alone configuration.

Economic Parameters	**Value**	**Reference**
Reference date	December 2019	Assumed
Project lifetime (years)	25	[12]
Linear depreciation rate (first 10 years)	10%	[49]
Working capital (% of FCI [a])	10%	[49]
Minimum acceptable rate of return	12%	[49]
Corporate income tax	25%	[49]
Social contribution on net income	9%	[49]
Location factor	1.3	[49]
Exchange rate	4.11 R$/USD	[58]
Prices		
Bagasse (USD/dry t)	20	[50]
Electricity (USD/MWh)	52.4	[50]
Natural Gas (USD/m^3)	0.62	[59]
Jet fuel (USD/L)	0.53	[57]
Anhydrous Ethanol (USD/L)	0.47	[60]
Fixed operating costs		
Average cost per employee [b] (USD/month), 2G	1268	[61]
Number of employees, 2G	30	[12]
Average cost per employee [a] (USD/month), 1G	1174	[61]
Number of employees, 1G	320	[49]
Insurance (% of FCI)	0.7%	[62]
Annual maintenance (% of FCI)	3%	[49]

[a]: Fixed Capital Investment. [b]: Overhead and benefits included.

2.4. Environmental Assessment

The life cycle assessment followed the methodology described by ISO [63,64] and included all material flows and emissions from biomass production, industrial conversion, fuel distribution, and fuel use based on a well-to-wake approach. The environmental impacts among the multiple products were shared considering energy allocation. The background inventories were retrieved from ecoinvent database v3.4 [65]. The climate change impact was assessed in view of the global warming potential (GWP) within a 100-year time horizon according to the IPCC method [66]. In addition to climate change impacts, six other impact categories from the ReCiPe Midpoint (H) 1.06 method [67] were selected for comparison of standard aviation fuel and fossil jet fuel.

The methodology described by the RenovaBio policy [9] was adopted for calculation of carbon credits (Cbios) in each scenario. The Brazilian Stock Exchange started accepting trades of CBios in 2020 [68], and certified biofuel producers as well as importers can claim these credits. Each CBio corresponds to a reduction of one metric ton of CO_2 when comparing the emissions of biofuels against their fossil counterparts. The calculation of the number of credits takes into account the produced volume of the biofuel and the emission index [9,69]. This index, also defined as avoided emissions of CO_2-eq, consists of the difference between the GHG emissions of fossil fuel and of renewable fuel. The avoided emissions of a particular biofuel production process, conforming to the RenovaBio policy, are calculated and verified by third-part entities for issuing certification to producers. This estimation is based on the life cycle assessment of the production chain, with a cradle-to-grave approach. Equations (1) to (3) show the method for the calculation of the revenues obtained with Cbios credits. The carbon price assumed was USD 10 per metric ton of CO_2-eq avoided [70].

$$Avoided\ emissions_{SAF}\left(\frac{tCO_{2\ eq}}{MJ}\right) = GHG\ emissions\left(\frac{tCO_{2\ eq}}{MJ}\right)_{fossil\ jet\ fuel} - GHG\ emissions\left(\frac{tCO_{2\ eq}}{MJ}\right)_{SAF} \tag{1}$$

$$Cbios_{credit}(tCO_2) = Avoided\ emissions_{SAF}\left(\frac{tCO_{2eq}}{MJ}\right) \cdot Volume\ produced_{SAF}\ (MJ) \tag{2}$$

$$Cbios_{revenue}(\$) = Cbios_{price}\left(\frac{\$}{tCO_2}\right) \cdot Cbios_{credit}(tCO_2) \tag{3}$$

The baseline value adopted for GHG emissions of fossil jet fuel was 87.5 gCO_2-eq/MJ, following the premises of the RenovaBio policy [71]. By deducting HTL SAF emissions from fossil jet fuel emissions, it was possible to calculate the avoided emissions (Equation (1)). This value was multiplied by the produced volume of sustainable aviation fuel to obtain the amount of Cbios credit (Equation (2)). Finally, the amount of Cbios credit was multiplied by Cbios price to obtain the revenue with Cbios in each of the evaluated scenarios (Equation (3)).

2.5. Uncertainty Analysis

A Monte Carlo analysis was carried out with 10,000 runs for each of the assessed scenarios to test the robustness of our method. The inputs for the risk analysis were selected considering the most influential parameters, as shown in Table 4. Among these, the HTL bio-crude oil yield variable is key to the results generated. In this study, this yield was assumed to be only lower than the deterministic value (40.9% for the scenarios with water as solvent and 48.3% for the scenarios with ethanol). This assumption was based on the discussions from the literature regarding a likely decrease in bio-crude yields when moving from bench to industrial scale due to a possible overestimation of the reported yields in experimental studies [17,72]. The decreased range was adopted from a study that conducted HTL upscaling experiments [52]. The sugarcane production yield represented the uncertainty related to the production cost of sugarcane stalks and straw, which directly affects the final cost of biomass, and, indirectly, the transportation distance and the corresponding GHG emissions. For the sugarcane bagasse, the opportunity cost range was obtained from the SUCRE project [50].

Table 4. Main parameters adopted for the uncertainty analysis.

Parameters	Deterministic Value	Min.–Max.	Probability Distributions
Sugarcane yield (ton/ha)	80	69–86	Triangular
Bio-crude yield, EtOH (%)	48.3	38.6–48.3%	Uniform
Bio-crude yield, H_2O (%)	40.9	32.7–40.9%	Uniform
CAPEX HTL (%)	Calculated	90–130%	Triangular
CAPEX 1G distillery (%)	Calculated	90–130%	Triangular
Location factor	1.3	1.0–1.3	Uniform
MAAR (%)	12	10–12%	Triangular
Bagasse cost (USD/dry ton)	10	4–21	Triangular
Natural gas price (USD/m^3)	0.57	0.47–0.68	Triangular
Cbios price (USD/t)	10	3–39	Triangular
Jet fuel price (USD/GJ)	16.2	13.9–18.5	Triangular
Transportation distance (km)	36.1	10–63	Triangular

For the minimum attractive rate of return (MAAR), the uncertainties that were taken into account are related to the capital cost and risk volatility associated with investments in new technologies in the sugarcane industry. The uncertainties related to the estimation of capital investment followed a variation reported elsewhere [49].

The location factor has either a deterministic value (that considers the additional CAPEX in Brazil, which is 1.30 times the cost estimate in the U.S.) or a value that relies on the possibility that the equipment could be manufactured nationally. If this were the case, it would be a multiplier factor of 1 [73]. The price range for the chemical inputs and products was retrieved from the last ten years' historical average [57,59]. The Cbios historical prices were obtained from the bids but with a shorter historical reference since the trade of Cbios in the stock exchange started in 2020 [69,70].

3. Results and Discussion

3.1. Techno-Economic Analysis

Figure 2 shows the results obtained from the techno-economic analysis for the different scenarios. The capital expenditures (CAPEX, Figure 2a) are in the range of USD 237–259 million for the stand-alone scenarios, and USD 542–554 million for the integrated scenarios. However, the capital cost per metric ton of processed biomass of the stand-alone scenarios was USD 5 million, that is, much higher than the value for the integrated scenarios, which is the first evidence of the better performance of the integrated configuration. The most representative units in terms of capital expenditures were liquefaction, upgrading, biodigestion, steam and power generation, and 1G ethanol distillery.

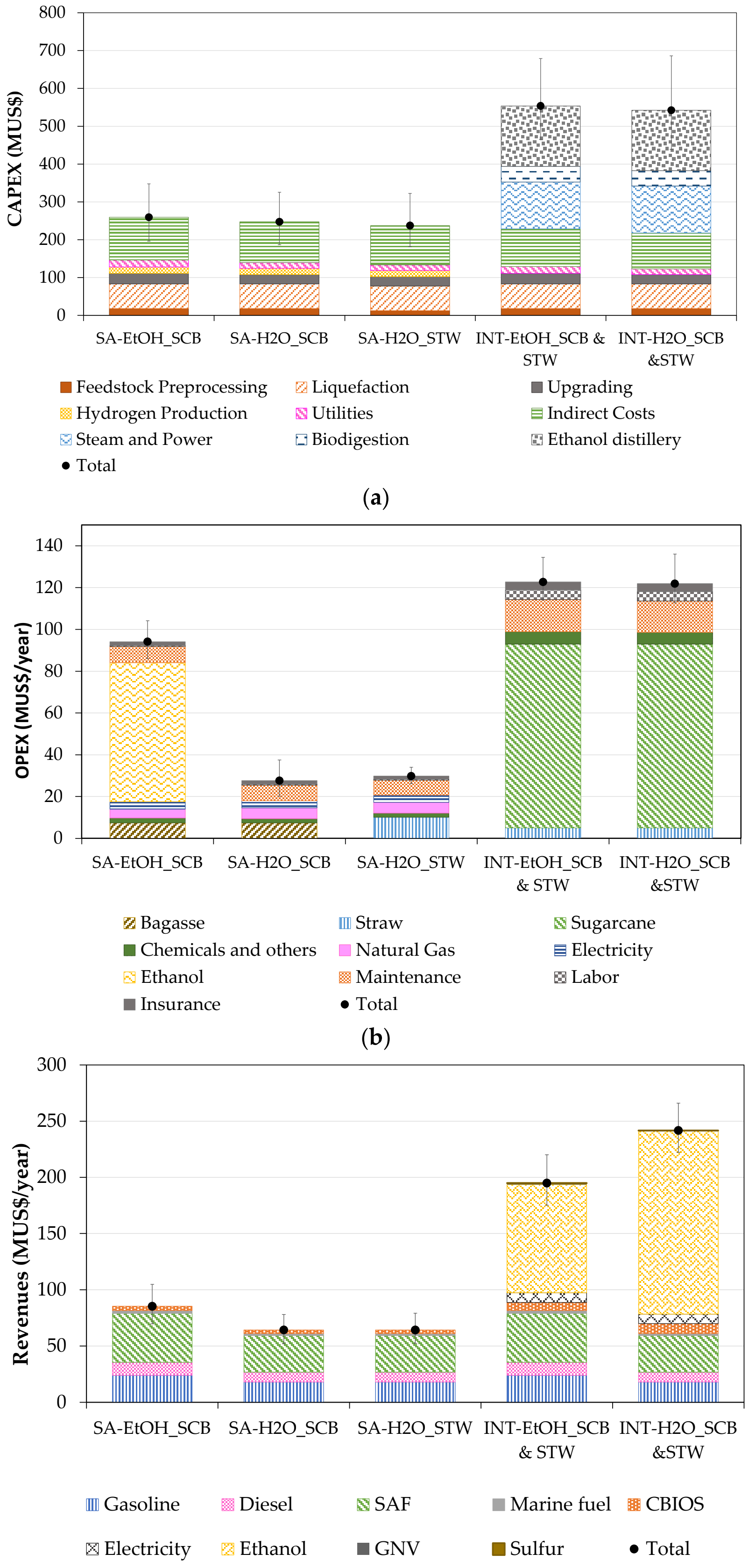
Regarding uncertainties associated with the economic outputs displayed in Figure 2, those associated with capital costs (Figure 2a) are much more prominent compared to both the operational costs (Figure 2b) and the revenues (Figure 2c). For instance, the capital investment in the integrated scenarios can reach ca. USD 700 million. This is because HTL has not yet fully reached technological maturity; thus, robust data of HTL equipment at commercial scale are still unavailable in the literature. The uncertainties related to location factor, i.e., the impacts of either paying extra costs of HTL equipment from abroad or relying on the possibility of national manufacture of the equipment, also play an important role in the results for the CAPEX. Therefore, this uncertainty is higher in scenarios with higher overall capital costs. Other studies have also identified the capital investment as a key parameter related to economic uncertainty of the HTL process [74,75].

Figure 2b provides the breakdown of operational expenditures (OPEX). Sugarcane straw is more costly than sugarcane bagasse on a mass basis; thus, the total operational cost of the SA-H_2O_STW scenario was 8% higher compared to the that of SA-H_2O_SCB scenario, whereas other inputs had a similar share amongst these two scenarios (except for ethanol as solvent). The uncertainties related to the OPEX had a modest margin of variation and were mostly affected by biomass cost (for bagasse) and yield (for straw). Comparing the uncertainty range between the stand-alone scenarios, lower values for SA-H_2O_STW were observed since the uncertainty variation related to the sugarcane straw yield was smaller than the one related to the cost of sugarcane bagasse. The operating expenses were very similar in the integrated scenarios and the main costs were associated with the biomass feedstock (sugarcane stalks and straw). In the INT-EtOH_SCB & STW scenario, ethanol for liquefaction reactions was obtained from the ethanol distillery instead of being purchased.

Figure 2c shows the breakdown of the annual revenues. Those related to sustainable aviation fuel (SAF) had the highest share in the stand-alone scenarios and represented the second highest contribution in the integrated scenario. The revenue associated with the selling of ethanol played a very significant role, as expected, thus representing 67% of the incomes in the best scenario (INT-H_2O_SCB & STW). The magnitude of this contribution has to do with the fact that the first-generation ethanol production has a fully developed level of technological maturity, along with a very well-established market. The carbon credits (Cbios) have contributed to the revenue in all scenarios. For the stand-alone scenarios, it ranged from USD 3.1 to 3.8 million per year, thus representing 4.4–4.8% of the total revenues. For the integrated scenarios, the annual contribution with Cbios was USD 7.3–8.7 million, representing a share of 3.7–3.9% of the total revenue. Among all cases, the highest contribution from Cbios was observed in the integrated scenarios due to the commercialization of first-generation ethanol. The higher revenues from SA-EtOH_SCB (among the stand-alone scenarios) were offset by the excessive costs associated with the acquisition of ethanol for the liquefaction reactions.

It is important to stress the importance of vinasse biodigestion unit in the integrated scenarios. Although it accounts for additional USD 41 million in the total CAPEX, the savings associated with the avoided purchase of natural gas amounted to around USD 25 million every year. The biomethane surplus (excess obtained after the reform into hydrogen) was assumed to be upgraded and sold as vehicular natural gas (VNG). Similarly, we took into account that sulfur recovered after biomethane desulfurization also contributed to the total revenues.

Figure 3 shows the main results from the discounted cash flow analysis, whose values point to the advantage of the integrated scenario with water (INT-H_2O_SCB & STW) in terms of achieving economic feasibility. In fact, this scenario allows both positive net present values and positive NPV/CAPEX (Figure 3a,b). As shown in Figure 3, the other scenarios do not point to economic feasibility even when considering the best results from the uncertainty analysis. Moreover, it is noteworthy to mention that the internal rate of return of the INT-H_2O_SCB & STW scenario (Figure 3e) has more than 75% chance of being above 10% per year, which is the common rate adopted in similar studies carried out in the literature in countries with lower risk [12,29,76]. The IRR of SA_EtOH_SCB is not displayed in Figure 3e because it could not be determined for most of the runs of the uncertainty analysis. This is because this scenario demonstrated very poor economic performance, thus resulting in negative or indeterminate values of IRR. Figure 3c shows a significant discrepancy between the stand-alone scenario with ethanol (SA-EtOH_SCB) and the other scenarios, since its payback time can be as high as 50 years, twice the lifetime of the HTL project.



(**a**)

(**b**)

(**c**)

Figure 2. Economic results: (**a**) CAPEX (MUSD), (**b**) OPEX (MUSD/year), and (**c**) revenues (MUSD/year).

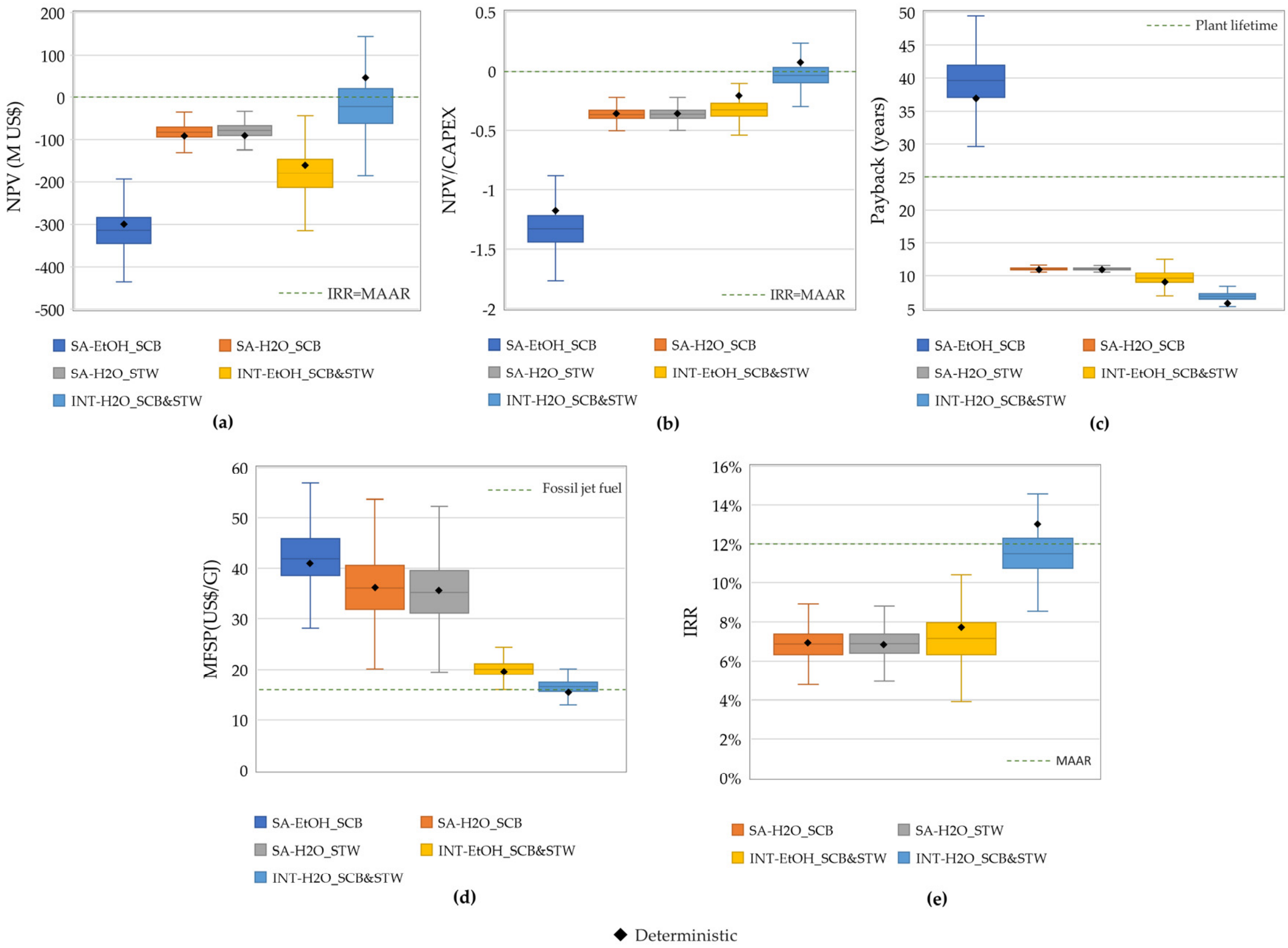


Figure 3. Results from the discounted cash flow analysis based on the Monte Carlo analysis: (**a**) NPV (MUSD/year), (**b**) NPV/FCI, (**c**) payback (years), (**d**) SAF MFSP (USD/GJ), and (**e**) IRR (%).

Figure 3d presents the minimum selling price of SAF from different scenarios, an important metric for biofuel's techno-economic competitiveness. The deterministic values MFSP in the stand-alone scenarios were in the range of 35–41 USD/GJ SAF, in accordance with the values found in the literature of 21–60 USD/GJ [11,29,77]. For the stand-alone scenarios, the most influential parameters were the discount rate, capital costs, bio-crude yield, and carbon credit prices. The lowest MFSP was 15.4 USD/GJ, observed in the integrated scenario (INT-H_2O_SCB & STW). This value is slightly lower than the fossil jet fuel price of 16.2 USD/GJ, indicating a very high competitiveness for this biorefinery configuration. Such a sharp reduction in the SAF production costs in the integrated scenario can be explained by a more balanced structure of costs and revenues, since the high capital investment associated with HTL equipment is diluted when integrated into the ethanol biorefinery. This potential benefit from integrating a thermochemical facility into a higher technology readiness level (TRL) biorefinery has also been demonstrated by de Jong et al. [29]. However, when the uncertainties associated with the parameters critical to this integrated scenario (INT-H_2O_SCB & STW) are taken into account, there is only a 38% probability of SAF reaching minimum selling prices lower than that of fossil jet fuel.

3.2. Life Cycle Assessment

Figure 4a shows the breakdown of GHG emissions related to the production, distribution, and use of HTL SAF. In the SA-EtOH_SCB scenario, the ethanol used as solvent corresponded to 47% of the total emissions. Although this scenario presents potential for GHG emission reduction of ca. 73% compared to fossil jet fuel, a lower environmental performance is observed when compared to the other scenarios. This clearly shows the dominance of water as a liquefaction solvent, while the utilization of organic solvents may represent a significant penalty to climate change impacts of HTL biofuels. This finding is in consonance with the results from the techno-economic analysis, which also highlight the disadvantages of using ethanol for HTL reactions (SA-EtOH_SCB and INT-EtOH_SCB & STW).

The industrial emissions originate from three different processes: combustion, steam methane reform, and biomethane production. In the stand-alone scenarios, the emissions are related to combustion (of biochar and off-gases) and hydrogen production through SMR. In the integrated scenarios, the emissions are related to combustion (of bagasse and straw) and biomethane production through vinasse biodigestion. Biofuel upgrading was an important contributor to GHG emissions in stand-alone scenarios, which are mostly related to the production of hydrogen by SMR (13–29% of the total emissions). The combustion of biochar and off-gases had only a marginal contribution during this stage (2–3% of the total emissions). The stand-alone scenario with ethanol (SA-EtOH_SCB) presented lower impacts from natural gas production and use compared to the scenarios with water (SA-H_2O_SCB e SA-H_2O_STW), since ethanol as a liquefaction medium results in a greater quantity of off-gases in the HTL process. These, in turn, are used as feedstock in the steam methane reform, thus decreasing the necessary amount of purchased natural gas in addition to lowering their impacts since off-gases emissions are partially regarded as biogenic. The production of natural gas (9–20% of the total emissions) and electricity (13–23% of the total emissions) also played an important role in stand-alone scenarios. A lower share of climate impacts is associated with the use of chemicals, infrastructure, and biomass. In the stand-alone scenarios, the impacts associated with production of chemicals are mainly related to the catalysts (for the bio-crude upgrading and SMR) and wastewater treatment. In the case of bagasse used as feedstock for HTL SAF, this study assumes that the life cycle GHG emissions are burden-free, according to the RenovaBio framework policy, which is in line with directives from the EU parliament [3,9]. Therefore, only the impacts due to the bagasse transportation are considered. The impact associated with the sugarcane straw was mainly due to harvesting operations and transport emissions, so climate impacts per kilogram of straw are slightly higher compared to the same amount of bagasse. Overall, the impacts associated with the HTL conversion stage are the most significant in the stand-alone scenarios, with a contribution in the range of 74–83%.

Regarding the integrated scenarios, biomass production has the most significant share of the impact, ranging from 63 to 64% of the total emissions. The climate impacts from sugarcane comprise all the agricultural operations related to cultivation, harvest, and transport to the conversion plant. Compared to the stand-alone scenarios, these emissions are also much higher due to larger production scales in the integrated scenarios. Per year, while HTL stand-alone scenarios process 0.37 million metric tons of either bagasse or straw, the integrated scenarios have an input of 4 million metric tons of sugarcane stalks. Besides biomass, the fuel distribution stage makes the second largest contribution to the GHG emissions (a share in the range of 17–19% of the total emissions), mostly because of the definitions from the RenovaBio framework, which establish a standard average distance of 1500 km by road transport from the biorefinery to the largest airports in Brazil [9,71]. Other important sources of GHGs are related to industrial emissions (6%), infrastructure (6%), and chemicals (3%). Differently from the stand-alone scenarios, there were no impacts related to background emissions from either electricity or natural gas production, since energy demand in the integrated scenarios is supplied by the CHP system and biomethane is produced internally. The industrial emissions are related to combustion of bagasse and straw, as well as to the biomethane production. Chemicals in the integrated scenario comprised all of those used in the different unit operations of first-generation ethanol, for the biomethane production and the HTL plant.

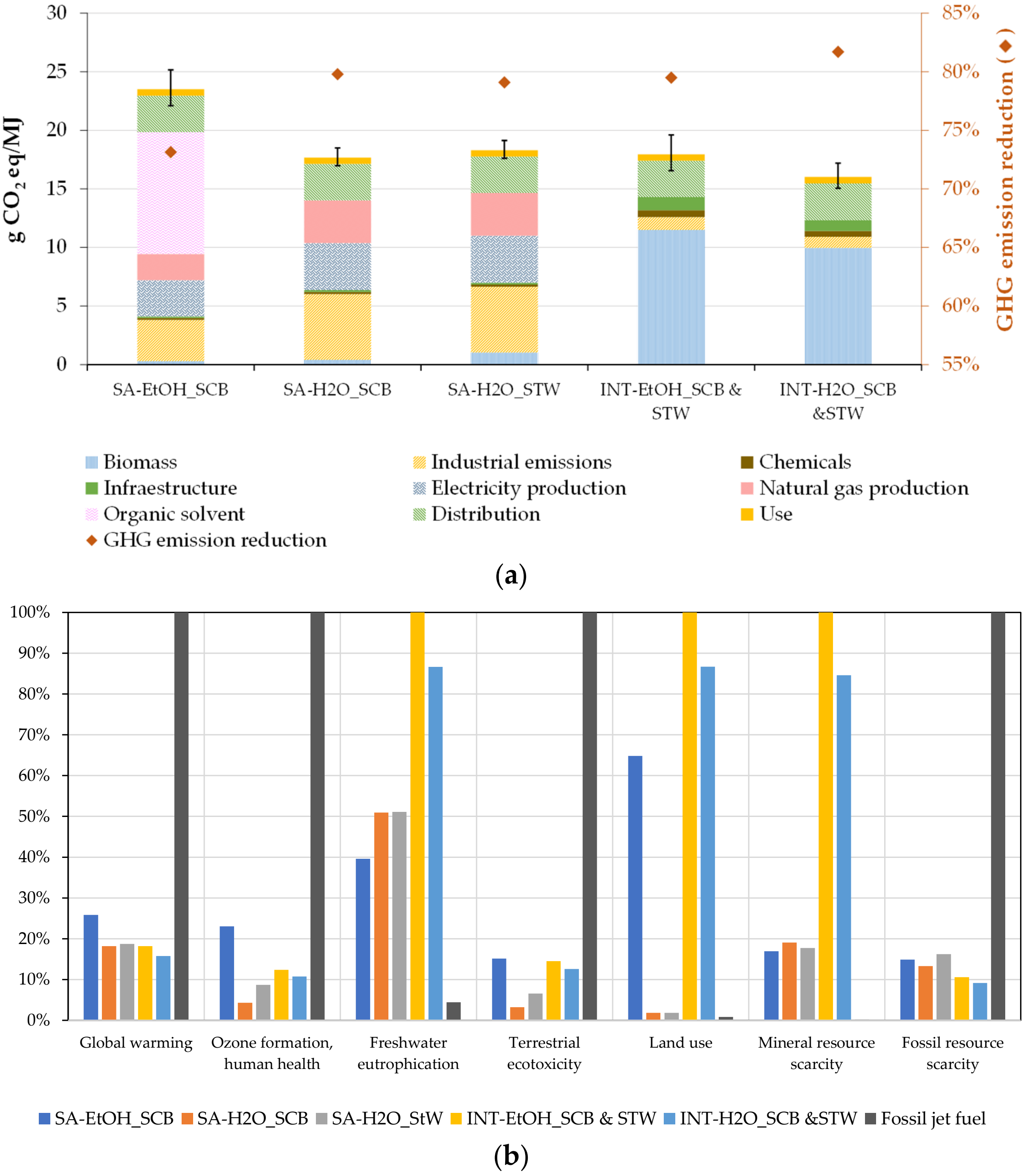


Figure 4. Environmental results of standard aviation fuel in the evaluated scenarios: (**a**) breakdown of GHG emissions, (**b**) selected impact categories.

The uncertainties associated with GHG emissions did not result in wide variations. In the stand-alone scenarios, these uncertainties are mainly affected by the bio-crude yield and the transport distance of biomass residues (sugarcane bagasse and straw). For the integrated scenarios, sugarcane productivity and the bio-crude oil yield are the main drivers of GHG emissions uncertainty because of their influence on the final outputs of the process.

For the other impact categories (Figure 4b), the HTL sustainable aviation fuels presented a better performance related to the global warming, ozone formation, terrestrial ecotoxicity, and fossil resource scarcity compared to the fossil jet fuel. The fossil jet fuel had a much more pronounced impact in the global warming category due to the fossil emissions in the combustion stage. The same trend was observed for the impact of ozone formation in human health, due to the emission of nitrogen oxides in the combustion of fossil jet fuel. In the categories of freshwater eutrophication, land use, and mineral resource scarcity, a poorer environmental performance was observed in the scenarios processing biomass. The freshwater eutrophication is mainly related to the emissions of the phosphorus-rich nutrients that reach freshwater. The integrated scenarios presented a much higher impact in the land use category due to biomass production in the agricultural stage. The higher impacts of the SAF scenarios in the mineral resource scarcity category are attributed to the use of chemicals in the industrial stage. Another important outcome of this study is that the scenarios with ethanol as solvent presented higher impacts in almost all of the categories compared to the scenarios with water as solvent. For instance, in the land use category, the SA-EtOH_SCB scenario showed a much higher impact within the stand-alone scenarios because of the indirect land use required for sugarcane cultivation to produce ethanol used as solvent. The INT-EtOH_SCB&STW scenario also showed the worst environmental performance in all the categories compared to the integrated scenario using water as solvent. This is because these scenarios imply a significant amount of ethanol as solvent for the liquefaction reactions. The liquefaction of biomass is carried out using a high feedstock-to-solvent ratio (in the present study as high as 80% solvent and 20% biomass). Therefore, the input of ethanol (on a mass basis) is higher than the overall output of biofuels (in mass basis), even considering that the solvent is recovered and recirculated to the process with a make-up of 10% (on a mass basis). Therefore, even though the utilization of an organic solvent such as ethanol may produce better technical results in terms of bio-crude oil yield and quality, as extensively stated in the literature [25,26,28,78–82], this moderate enhancement results in a substantial penalty in terms of economic and environmental performance because of the disproportionate amount of ethanol as an input to the HTL process compared to both the biomass feed and the product output. Future literature should focus on investigating the utilization of solvents for the HTL downstream process instead, such as the addition of organic solvents to improve the HTL bio-crude quality and stability. This would allow for a much lower quantity of solvent as input to the process. More information regarding the share of the impacts in each of these categories, and in each of these scenarios, can be found in the Supplementary Material (Figures S6–S10).

3.3. Comparison of our Results with the Literature

Among all scenarios assessed in this study, the well-to-wake climate impacts are in the range of 16–24 gCO_2-eq per MJ of SAF. These results are in consonance with the literature, which reports values for lignocellulosic biomasses within a range of 13–21 gCO_2-eq/MJ SAF. In terms of industrial plant configuration, the stand-alone scenarios using water as solvent are more comparable to previous HTL studies available in the literature; therefore, we will focus on SA scenarios to deliver more consistent comparisons.

Tzanetis et al., Björnsson and Ericsson, and de Jong et al. [11,21,29] calculated the GHG emissions from HTL of forestry residues as 13, 20, and 21 gCO_2-eq/MJ SAF, respectively. Nie and Bi [22] obtained values of 17, 19.5, and 20.5 gCO_2-eq/MJ SAF, which were very close to those obtained in this study (17.7 and 18.3 gCO_2-eq/MJ SAF for SA-H_2O_SCB and SA-H_2O_STW, respectively). They also demonstrated that the industrial conversion stage was the most intensive in terms of GHG emissions, similar to the results obtained in the present study. However, climate change impacts associated with biomass production and industrial preprocessing had a significant share in their results, whereas contributions from these stages were relatively smaller in this study (Figure 4a). Such differences might be related to their different value chain structure comprising forestry management operations, equipment, and transport distances of residues when compared to ours, in this study. This shows the important role that feedstock plays in the results of environmental impacts. Despite these differences, both studies indicate a great potential of SAF to mitigate GHG emissions from fossil jet fuels.

Literature data frequently highlights that the contribution of the fuel distribution stage to the overall well-to-wake climate impacts is usually very low. In this study, however, it represents a relevant share of GHG emissions (13–18% of the total emissions in the SA scenarios). As previously discussed, the adopted fuel distribution distance of 1500 km (from the biorefinery to the airport) based on the RenovaBio standards is much higher than the range of 48–348 km reported in the literature [6,14,15,20]. Although our results present similarities to the overall climate impacts described in the literature, there are differences regarding the main contributors to the GHG emissions. Besides the variations in methodological assumptions for the life cycle assessment, there might be other variations associated, for instance, with both foreground and background inventory databases. In the present study, background data were based on ecoinvent, and some were adapted to better represent possible technological differences observed in Brazil [83].

Another key aspect of the HTL SAF climate impacts is related to hydrogen sourcing. Studies have reported a significant share of climate change impacts being associated with the use of natural gas as a feedstock for steam methane reform. In the integrated scenarios, the biomethane produced from the vinasse biodigestion reduced the GHG emissions in the production stage by 16–19%. The biodigestion of post-HTL aqueous phase in the scenarios using water as solvent could also represent an extra source of biomethane, thus lowering the overall impact. However, this process design option was not included in the present study.

Figure 4a also shows that the potential climate mitigation from HTL SAF is in the range of 73–82% when compared to fossil fuels. In the view of the Renewable Energy Directive II (RED II) definition of advanced biofuels, HTL SAF assessed in this study from sugarcane bagasse and straw can be considered as an advanced biofuel since its feedstock is based on biomass residues. According to the Renewable Fuel Standard (RFS) [84], a cellulosic biofuel (within the advanced fuel category) should reduce emissions by at least 50% in relation to fossil fuel and be derived from cellulose, hemicellulose, or lignin (non-food-based). These requirements were met in our scenarios, thus making HTL-based SAF of sugarcane residues also eligible as cellulosic biofuel based on U.S. standards. The advantage of using lignocellulosic biomasses, as shown in this study, is also clear when compared with other biomasses. Studies of HTL conversion from algae-based SAF, for instance, reported GHG emissions from 35 to 86 gCO_2-eq/MJ [85] and 44 gCO_2-eq/MJ [86]. These results would have a GHG reduction in the range of 1–60%, much lower than the climate mitigation potentials obtained in the present study.

3.4. Cbios

The economic feasibility of the HTL scenarios is sensitive to Cbio prices, as they lead to a 4–5% reduction in the MFSP for both stand-alone and integrated scenarios when compared to the baseline scenario without revenues from Cbios. The International Energy Agency projected that the carbon price in Brazil may reach 43 USD/metric ton in 2025 and 125 USD/metric ton in 2040 when considering a sustainable development scenario [87]. Based on this projection, the MFSP curves shown in Figure 5 consider a Cbio price that ranges from 10 USD (minimum RenovaBio historical prices) to a maximum of 125 USD. It is important to point out that none of the stand-alone scenarios would reach values comparable to the fossil jet fuel price, even when considering the highest prices from IEA's projection. On the other hand, the integrated scenario with ethanol (INT-EtOH_SCB & STW) shows a potential equivalence to the fossil jet price for a Cbio price above 70 USD/metric ton. However, it is important to remark that none of the scenarios are likely to become economically viable according to the uncertainty analysis, except for the integrated scenario with water (INT-H_2O_SCB & STW). Therefore, an aggressive increase in carbon prices would not be enough for these other scenarios to achieve economic feasibility.

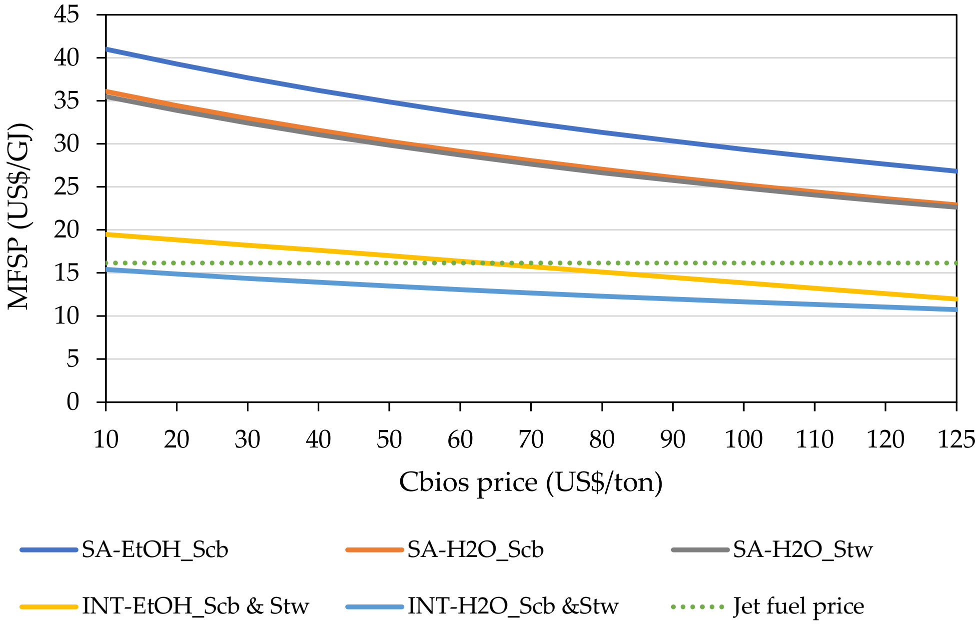


Figure 5. Influence of Cbios price on the MFSP of sustainable aviation fuel.

4. Conclusions

This study provides a unique contribution by presenting the economic and environmental metrics for the production of HTL-based SAF from sugarcane residues in Brazil. The results point to its potential feasibility considering not only GHG emission reduction, but also the minimum fuel selling price of SAF. The evaluated scenarios showed a reduction in GHG emissions in the range of 73–82% compared to fossil jet fuel, and notably the integrated scenario with water as the best environmental performance in terms of climate mitigation. Therefore, HTL SAF produced from sugarcane bagasse and straw can be regarded as an advanced fuel according to international regulations such as RED II and the RFS. The carbon credits associated with the RenovaBio policy contributed additional revenues in all the evaluated scenarios, lowering the minimum fuel selling price of SAF by up to 5%. However, this incentive alone was not enough to enable the economic viability of the stand-alone scenarios, even in light of very optimistic carbon credit scenarios at 125 USD/tCO_2-eq avoided. The results of the minimum selling price indicate that HTL SAF can be competitive with fossil jet fuel only if HTL is integrated into the first-generation sugarcane industry.

SAF production from HTL technology was shown to greatly benefit from the integration with ethanol distilleries as it resulted in lowering the overall capital and operational costs of the project. The uncertainty analysis showed that there is a 38% chance of HTL SAF reaching compatible prices with fossil jet fuel in the integrated scenario with water. In this scenario, the uncertainty analysis also demonstrated that there is a 75% chance of the internal rate of return being above 10% per year, thus showing the promising potential of this integration if a lower minimum attractive rate of return is taken into account. However, neither the stand-alone nor the integrated scenarios with ethanol (as solvent) have potential for economic feasibility at the current stage of the technology, even when optimistic premises for the key economic parameters were considered. The employment of ethanol as solvent for liquefaction reactions was demonstrated to significantly penalize the environmental performance of HTL biofuels, along with prohibitive costs, showing that the utilization of an organic solvent for liquefaction has no feasibility at large scale. Future studies should investigate the utilization of organic solvents at reasonable, lower proportions or investigate the utilization of organic solvents only for the upgrading stage in order to improve the bio-crude oil quality and stability.

The large-scale deployment of HTL SAF integrated into the Brazilian sugarcane industry may help achieve the GHG emission reduction established by CORSIA, which will be mandatory in the coming years. It will also be highly relevant for the accomplishment of the net-zero emission scenario by 2050, since the decarbonization of the aviation sector heavily relies on the commercialization of advanced fuels that are still at the demonstration stage. Although such integration suggests greater potential towards economic feasibility for HTL SAF production, improvements in the combination of the sugarcane industry and HTL technology can be further enhanced in Brazil by lowering interest rates, reducing capital costs, and incorporating government subsidies. It is important to remark that HTL SAF has not yet been certified by ASTM to be blended with fossil jet fuel. Studies concerning the compliance of the properties of HTL SAF with the standard requirements are still being carried out, and it is expected that the running tests performed by the existing HTL demonstration facilities will make an important contribution to this advancement.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/en16062723/s1, Table S1 Biomass characterization, Table S2 Heat and power factors for the calculation of mass and energy balances of HTL, Figure S1 Mass fluxogram of SA-EtOH_SCB, Figure S2 Mass fluxogram of SA-H_2O_SCB, Figure S3 Mass fluxogram of SA-H_2O_STW, Figure S4 Mass fluxogram of INT-EtOH_SCB&STW, Figure S5 Mass fluxogram of INT-H_2O_SCB&STW, Table S3 CAPEX of the stand-alone scenarios, Table S4 HTL CAPEX of the integrated scenarios, Figure S6 Environmental impact breakdown for the selected categories of SA-EtOH_SCB, Figure S7 Environmental impact breakdown for the selected categories of SA-H_2O_SCB, Figure S8 Environmental impact breakdown for the selected categories of SA-H_2O_SCB, Figure S9 Environmental impact breakdown for the selected categories of INT-EtOH_SCB&STW, Figure S10 Environmental impact breakdown for the selected categories of INT-H_2O_SCB&STW, Table S5 Life Cycle Inventory of the evaluated scenarios.

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